Electron-positron interaction in light elements represented by atoms embedded in an electron gas

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Mijnarends et al. [J. Phys. Condens. Matter **10**, 10383 (1998)] contested the best existing calculations of positron annihilation rates in jellium and crystal lattices, pointing in this way at deficiencies of existing theories of electron-positron interaction in these materials. In the present work the local enhancement factors due to $e^+ - e^-$ interaction in Li, Be, B, C, N and O are computed in a consequent many-body approach for core and as concerns lithium also for conduction electrons and compared to the results of existing approximations to this problem which avoid direct many-body calculations in metals, i.e. the local density, generalized gradient and weighted density approximations, as well as to experimental data. Conclusions about positron lifetime and $e^+ - e^-$ correlation energy are also presented. Suggestions concerning annihilation rates in an electron gas agree with those of Mijnarends et al.

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I. INTRODUCTION

The purpose of this work is a study of electron-positron interaction (EPI) in solids represented by an atom embedded in an electron gas. There are good reasons to believe that EPI in such a model gives valuable information on $e^+ - e^-$ interaction. Indeed, in most calculations the local annihilation rates are assumed to depend only on the local electron density, in generalized gradient approximation also on its local gradient[1]. In our work they are functionals of the whole electron distribution in an atom while the neighboring atoms are simulated by an averaged electron density and a constant positive background.

This model was used to compute the effect of EPI for light elements. However, the approach to electronic structure used in this work (i.e. presenting the population of valence electrons by means of a single density amplitude in the form proposed by Gondzik and Stachowiak[2]) seems to hold only for alkalis[3,4]. So more or less reliable calculations of the enhancement of valence electrons in these elements were performed only for lithium. As concerns other elements, we had to limit ourselves to core electrons for which the density amplitude is equivalent to the wave function.

The unknown effect of EPI on annihilation characteristics has always been considered as an obstacle in interpretation of annihilation data[5]. Nevertheless positron annihilation found many applications in studies of the solid state and in other domains (including biology, medicine and even marketing) and proved to give valuable information on electronic and ionic structures[6,7].

EPI in many electron systems has also been the subject of many investigations both theoretical and experimental. A review of different approaches to this problem is given in Ref. 8.

In particular, the unknown effect of the interaction of the positron with core electrons (IPC) introduces an uncertainty which is an obstacle in the interpretation of experimental data in terms of properties of valence electrons.

From the many attempts to estimate the effect of IPC (and EPI in general) on the annihilation data let us mention the local density approximation (LDA)[9,10], the generalized gradient approximation (GGA)[1], the weighted density approximation (WDA)[11] and others[12,13].

In the works[9,11] no attempt is performed to study the behavior of electrons in solids in presence of the positron basing on the equations of quantum mechanics. They all benefit of the results of jellium calculations. GGA takes into account the inhomogeneity of the medium, but has to introduce a phenomenological constant in order to get agreement with experimental measurements of positron lifetimes in metals. This agreement was contested as concerns other applications by Mijnarends et al.[14] who performed two-detectors Doppler broadening measurements in Al. WDA has the merit of enforcing a total charge of the screening cloud around the positron equal to one electronic charge.

Among the many-body calculations the most advanced are those of Sormann[13]. But even in them no attempt to reach self-consistency is undertaken.

In the present work we will develop the approach proposed by Gondzik and Stachowiak[2] in order to treat a positron in an electron gas and called mnemotechnically HNC (hypernetted-chain) following in that the work of Kallio et al.[15]. The approach of Ref. 2 is particularly simple, and leads to reasonable results. So one can hope that generalizing it to real solids will be easier than in the case of other approaches. The basic equations used in the present work have been proposed in Ref. 17 and the method of solving them for the anisotropic case (i.e. for the positron beyond the center of symmetry) is presented in Ref. 18. This work constitutes an application

of the methods elaborated in these last papers.

Indeed, some information about $e^+ - e^-$ interaction in lithium was already obtained along this line[16,17]. However, in these works we were unable to solve the occuring integro-differential equations in the two dimensions needed if the spherical symmetry is broken (it will be broken for the positron outside the nucleus). In the meantime a method to solve such equations was elaborated and then applied to lithium[18,19,20].

In this work we had to limit ourselves to light elements, since at present we are able to deal only with core electrons in the s orbital state. So we will perform calculations only for Li, Be, B, C, N and O.

The present state of the art can be characterized best basing on the recent enlightening work of Mijnarends et al.[14]. These authors interpret two-detectors Doppler broadening studies of Al in the following way.

They assume three models of $e^+ - e^-$ interaction which they label LDA, LDA' and GGA. The first two models apply the local density approximation to $e^+ - e^-$ interaction using the results of electron gas theory, in the first case those of Arponen and Pajanne (AP)[21], in the second case those of Lantto[22]. The third case corresponds to correcting the results of the local density approximation by adding a gradient correction to the enhancement factors of AP according to the work of Barbiellini et al.[1]. Mijnarends et al. find that the LDA' model gives the best agreement with experiment, though a small correction by applying a lesser than in Ref. 1 gradient correction could maybe lead to some improvement. These results illustrate the present state of knowledge of $e^+ - e^-$ interaction both in an electron gas and in real metals. Comparison of GGA with experiment performed in Ref. 14 led to disagreement.

As concerns deviations of enhancement factors from the local density approximation in metal lattices, this problem according to Ref. 14 is of lesser importance. But this conclusion follows from experimental considerations and means that a satisfactory theory of $e^+ - e^-$ interaction in metal lattices is not existing in spite of more than thirty years of research in this direction. Moreover, the LDA' model is based on the calculations of Lantto which assume an oversimplified trial function of the Jastrow type. This trial function neglects as well momentum dependence of $e^+ - e^-$ scattering and dependence of $e^- - e^-$ correlations on the distance from the positron - effects well established in physics and included in other calculations[21,23,24,25].

II. COMPUTATIONS

The model

Applying the approach of Gondzik and Stachowiak[2] to the problem of positron screening in an electron gas, we describe the electronic structure of an atom with two electrons core embedded in jellium with two functions $\psi_1(r)$ and $\psi_2(r)$. $\psi_1(r)$ is the wave function of core electrons and $\psi_2(r)$ is the density amplitude of valence electrons. $\psi_2^2(r)$ is equal to the density of conduction electrons in the model. These two functions obey the appropriate Kohn-Shamlike equations (in atomic Hartree units which will be used throughout the paper):

$$[-\tfrac{1}{2}\nabla^2 + V(\mathbf{r})]\psi_1(\mathbf{r}) = E_1\psi_1(\mathbf{r}),$$

$$[-\tfrac{1}{2}\nabla^2 + V(\mathbf{r})]\psi_2(\mathbf{r}) = 0 \qquad (1)$$

where

$$V(\mathbf{r}) = -\frac{Z}{r} + 2\int d\mathbf{r}'\frac{\psi_1^2(\mathbf{r}')}{\mid \mathbf{r}-\mathbf{r}' \mid} + \int d\mathbf{r}'\frac{\psi_2^2(\mathbf{r}') - d(\mathbf{r}')}{\mid \mathbf{r}-\mathbf{r}' \mid} + V_{HL}\{2\psi_1^2(\mathbf{r}) + \psi_2^2(\mathbf{r})\} - V_{HL}\{\rho_0\}. \qquad (2)$$

Z is the charge of the nucleus, $d(\mathbf{r})$ is the distribution of the positive charge in the electron gas. It is equal

$$d(r) = \begin{cases} \rho_0 & \text{for} \quad r > R_{WS}, \\ 0 & \text{for} \quad r < R_{WS} \end{cases} \qquad (3)$$

where

$$\rho_0 = D\frac{3(Z-2)}{4\pi(R_{WS})^3}. \qquad (4)$$

R_{WS} is the radius of the Wigner-Seitz sphere. Eqs. (1) – (2) limit us to elements having a two-electrons core. $V_{HL}\{\rho\}$ is the Hedin-Lundqvist exchange-correlation correction for an electron gas of density ρ[26]. The Lagrange multiplier E_2 which should occur on the right-hand side of the second equation (1) is normalized to zero by the last term in the formula (2), while E_1 is the energy eigenstate of core electrons.

We admit, of course, that from the elements treated in this work only lithium can be described as above[3,4]. But since core electrons are only weakly affected by valence electrons, the way of presenting the electronic structure of these lasts is of little importance for our purpose. In fact in this work we used different ways of approximating the electronic structure of valence electrons, but this had a negligible influence on IPC.

D was chosen in order to satisfy the obvious normal-

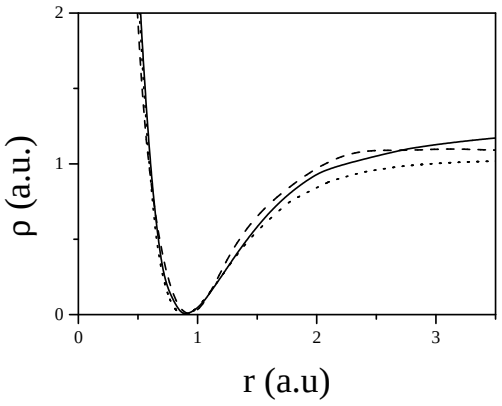

FIG. 1: Comparison of the density of valence electrons for a lithium atom in an electron gas - full curve for $D = 1.24$ and dotted curve for $D = 1$ and the analogous density (averaged over direction) for metallic lithium in HNC approximation[3] dashed curve.

ization condition

$$4\pi \int_0^{R_{WS}} r^2 dr \psi_2^2(r) = Z - 2. \tag{5}$$

This requirement could be satisfied for lithium where the value $D = 1.24$ leads to satisfying Eq. (5) and in beryllium where the value $D = 1.1$ was obtained. In Fig. 1 the distribution of valence electrons $\psi_2^2(r)$ is shown for $D = 1.24$ and compared to the distribution of valence electrons in metallic lithium obtained in HNC formalism[3] after averaging over directions. It is visible that the value $D = 1.24$ reproduces better the electron distribution in the immediate neighborhood of the atom.

Introduction of the positron

We benefit of the result obtained according to the theory of liquids by Kallio et al.[15] and concerning the role of the light mass of the positron in EPI. This suggests to describe the electronic structure of the model in presence of a positron at $\mathbf{r}_p$ by means of the equations

$$\left[-\frac{1}{2}\nabla^2 + V(r) + \frac{1}{2}W(\mathbf{r}_p, \mathbf{r})\right] \chi_1(\mathbf{r}_p, \mathbf{r}) = E_1(r_p)\chi_1(\mathbf{r}_p, \mathbf{r}),$$

$$\left[-\frac{1}{2}\nabla^2 + V(r) + \frac{1}{2}W(\mathbf{r}_p, \mathbf{r})\right] \chi_2(\mathbf{r}_p, \mathbf{r}) = 0 \tag{6}$$

where the screened electron-positron potential $W(\mathbf{r}_p, \mathbf{r})$ is defined as

$$W(\mathbf{r}_p, \mathbf{r}) = -\frac{1}{\mid \mathbf{r} - \mathbf{r}_p \mid} + W_p(\mathbf{r}_p, \mathbf{r}) + W_{xc}(\mathbf{r}_p, \mathbf{r}). \tag{7}$$

Here

$$W_p(\mathbf{r}_p, \mathbf{r}) = 2\int d\mathbf{r}' \, \frac{\chi_1^2(\mathbf{r}_p, \mathbf{r}') - \psi_1^2(\mathbf{r}')}{\mid \mathbf{r} - \mathbf{r}' \mid} + \int d\mathbf{r}' \, \frac{\chi_2^2(\mathbf{r}_p, \mathbf{r}') - \psi_2^2(\mathbf{r}')}{\mid \mathbf{r} - \mathbf{r}' \mid}, \tag{8}$$

$$W_{xc}(\mathbf{r}_p, \mathbf{r}) = V_{HL}\{2\chi_1^2(\mathbf{r}_p, \mathbf{r}) + \chi_2^2(\mathbf{r}_p, \mathbf{r})\} - V_{HL}\{2\psi_1^2(\mathbf{r}) + \psi_2^2(\mathbf{r})\}. \tag{9}$$

χ_i indicate the form of the functions ψ_i in presence of the positron. The positron distribution is described, of course, by the positron wave function.

Since the dependence of IPC on the perturbation of valence electrons by the positron is negligible, the equation for χ_1 can be solved separately. However, we consider as a better approximation to solve exactly the equations (6) for the easy problem of the positron on the nucleus and to compute χ_1 from the equation

$$\left[-\frac{1}{2}\nabla^2 + V^1(\mathbf{r}) + \frac{1}{2}W^1(\mathbf{r}_p, \mathbf{r})\right] \chi_1(\mathbf{r}_p, \mathbf{r}) = E_1(r_p)\chi_1(\mathbf{r}_p, \mathbf{r}). \tag{10}$$

Since the positron in metals is always screened by valence electrons, we found that when computing χ_1 it would be appropriate to freeze the valence electrons in the state they acquire for the positron on the nucleus. This will allow to determine the potentials V^1 and W^1 in Eq. (10). This equation will be solved afterwards for all values of $\mathbf{r}_p$.

Let us compute the solution of Eq. (6) for the positron on the nucleus, assuming that the core is frozen. We get in this way the potential

$$Q(\mathbf{r}) = \int d\mathbf{r}' \frac{\chi_2^2(0,r') - \psi_2^2(r')}{|\mathbf{r} - \mathbf{r}'|} + V_{HL}\{2\psi_1^2(r) + \chi_2^2(0,r)\} - V_{HL}\{2\psi_1^2(r) + \psi_2^2(r)\}. \tag{11}$$

The potentials in Eq. (10) can now be written in the form

$$V^1(r) = V(r) + \frac{1}{2}Q(r), \tag{12}$$

$$W^1(\mathbf{r}_p,\mathbf{r}) = -\frac{1}{\mid \mathbf{r}-\mathbf{r}_p \mid} + 2\int d\mathbf{r}' \frac{\chi_1^2(\mathbf{r}_p,\mathbf{r}') - \psi_1^2(r')}{\mid \mathbf{r}-\mathbf{r}' \mid}$$

$$+ V_{HL}\{2\chi_1^2(\mathbf{r}_p,\mathbf{r}) + \chi_2^2(0,r)\} - V_{HL}\{2\psi_1^2(r) + \chi_2^2(0,r)\}. \quad (13)$$

Solution of the equations

From test calculations it follows that the effect of positron interaction with conduction electrons depends only slightly also on the polarization of the core by the positron. So the equation for χ_2 can be solved separately.

The functions χ_i are presented in the form

$$\chi_i(\mathbf{r}_p,\mathbf{r}) = A_i(r_p)e^{-\alpha s} + \tau_i(\mathbf{r}_p,\mathbf{r}) \quad (14)$$

where the function

$$\tau_i(\mathbf{r}_p,\mathbf{r}) = \sum_{n=0}^{\infty} \varphi_n^i(r_p,r)P_n(\cos\vartheta) \quad (15)$$

is devoid of the cusp occuring in χ_i at the positron. $P_n(\cos\vartheta)$ are Legendre polynomials where ϑ is the angle between $\mathbf{r}$ and $\mathbf{r}_p$, $s = \mid \mathbf{r}-\mathbf{r}_p \mid$. From the assumption

$$\tau_i(\mathbf{r}_p,\mathbf{r}_p) = 0 \quad (16)$$

(the simplest one but not necessarily the only possible) it follows that $\alpha = 1/2$.

We have to limit ourselves for technical reasons to two terms in the expansion (15). This leads to some problems especially for higher values of r_p. They are discussed in more detail in Ref. 18.

The contact densities of electrons on the positron are provided by the $A_i(r_p)$ coefficients. An important information is also contained in the energy eigenvalue $E_1(r_p)$. Since $2E_1(r_p)$ will enter the positron Hamiltonian as a contribution to the positron potential, this quantity can be interpreted as effective attraction (of chemical character) between the positron and the nucleus due to collectivization of core electrons.

III. RESULTS

We were able to obtain numerical values for local annihilation rates of positrons in lithium. The results are shown on the figures. For other light elements we were able to study the effect of the interaction of the positron with atomic cores.

We call LDA the local density approximation, mentioning each time what results are used for describing the properties of a homogeneous electron gas: the ones of Gondzik and Stachowiak[2] or PHNC[25] (eventually the formula of Boroński and Nieminen (BN)[31]). Since the interactions of the positron with conduction and with core electrons can be to a large degree considered as independent, we introduce the term *local partial density approximation* (LPDA) which means that only core electrons or only conduction electrons (depending which electronic state is studied) contribute to the local density.

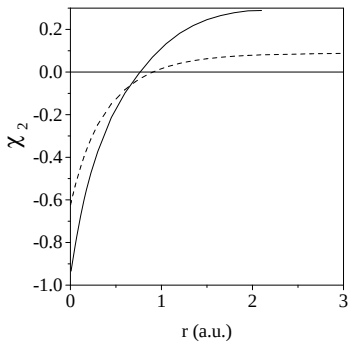

FIG. 2: The density amplitude of valence electrons in lithium as seen by positrons $\chi_2(r_p,r_p)$ (full curve) compared to the true density amplitude $\psi_2(r_p)$ (dashed curve).

Note that the enhancement factors following from Eqs. (6) are approximate as concerns conduction electrons since they neglect the difference of scattering on the positron (and also on the nucleus) by different electronic states. This is why it is appropriate to compare them while using LPDA with the results of the Gondzik-Stachowiak approach. This problem does not occur in the case of core electrons.

The enhancement factors for core ($i = 1$) and for valence electrons ($i = 2$) are given by the square of the enhancement amplitude w_i which is defined as

$$w_i(\mathbf{r}_p) = \frac{A_i(\mathbf{r}_p)}{\psi_i(\mathbf{r}_p)} \quad (17)$$

On Fig. 2 the density amplitude as seen by positrons $\chi_2(r_p,r_p)$ is compared to the real density amplitude $\psi_2(r_p)$.

The enhancement amplitude of conduction electrons calculated according to (17) agrees quite well with LPDA predictions at $r_p = 0$. Also for r_p much bigger than the position of the node in ψ_2 it approaches the LPDA value. Note, however, that for big r's its value is higher than expected on ground of the local density approximation. We can interpret this effect as a result of increasing electron density between (approximately) the position of the node in ψ_2 and $r < 2.5$. This result is confirmed by the recent calculations of Boroński and Stachowiak[27] who study the possibility of applying a grid method for problems of that kind. A similar effect has been observed for vacancies[18] where a maximum of the enhancement factor occurs in the region of increasing electron density. In the present case we rather attribute this effect to the lack of periodicity of the model. In the intermediate region $A_2(r_p)$ is greatly affected by the displacement of the node (from 0.9 to 0.76 a.u.) due to interaction with the positron.We consider this effect as very important, impossible to obtain using other approaches to EPI. Such an effect has been observed experimentally by Chiba in MgO[28].

The enhancement amplitude for core electrons is presented in Fig. 3a for Li. Remark that in the immediate vicinity of the nucleus the enhancement amplitude is a little bigger than LPDA predictions, while for higher values of r it falls below the LPDA curves.

Fig. 3b shows that the effective enhancement for lithium defined as

$$\varepsilon(r_p) = w_{eff}^2(r_p) = \frac{2A_1^2(r_p) + \tilde{A}_2^2(r_p)}{2\psi_1^2(r_p) + \psi_2^2(r_p)} \qquad (18)$$

reproduces quite well LDA predictions. $\tilde{A}_2(r_p)$ has been obtained from $A_2(r_p)$ by renormalizing it, taking account of the increasing error while r_p increases when solving Eqs. (6) and the deviation of the approximation of Ref. 2 from the exact value assumed to correspond to PHNC[25].

Of course, the local enhancement factor presented in Fig. 3a as well as the local enhancement of conduction electrons influence not only the positron lifetime but also angular correlation results.

As concerns the energy of $e^+ - e^-$ correlation E_{+-}, one can assume that conduction electrons give to it a constant (independent of r) contribution E_v, while the contribution of core electrons is provided by $2E_1(r_p)$. In Fig. 4a we compare $E_{+-} = 2E_1(r_p) + E_v$ to the appropriate predictions of LDA for the energy of $e^+ - e^-$ correlation. The jellium values were chosen according to PHNC[29].

In Fig. 4b we compare the positron wave function in lithium calculated using the LDA approximation for the $e^+ - e^-$ correlation potential to the wave function obtained when the effect of correlation was estimated according to our results.

We found also total annihilation rates for these two cases. We used the LDA approximation for the enhancement factor estimating that in the light of Fig. 3b it is quite justified. In the first case, when we applied the LDA approximation to the PHNC enhancement factor (using the PHNC formula[25]) and to the $e^+ - e^-$ correlation potential (with the formula from Ref. 29) we obtained a total annihilation rate of 3.63 $10^9/s$. The electron densities were calculated on base of the FLAPW (full potential linearized plane wave) method (the corresponding numerical code was WIEN95[30]).

The bigger penetration into the core region by the positron as shown in Fig. 4b results in slightly higher annihilation rates than in LDA because of high electron densities inside the core. Thus, for the potential calculated according to this work, the corresponding rate was 3.68 $10^9/s$.

The calculations performed with the BN enhancement[31] and the LDA correlation potential give a rate of 3.36 $10^9/s$. On the other hand, the calculations performed with the BN enhancement and our correlation potential give a rate of 3.42 $10^9/s$, what is accidentally in perfect agreement with experiment. The experimental annihilation rate for lithium is equal 3.436 $10^9/s$[32].

When calculating the positron wavefunction we used the numerical program by M. Puska[33] based, in principle, on superposition of atomic densities. We changed it slightly, however, in order to have the possibility to use electron densities and potentials calculated within the FLAPW method. Moreover, we generalized it on an arbitrary non-LDA $e^+ - e^-$ correlation potential. Note that Puska himself obtained an annihilation rate of 3.28 $10^9/s$ basing on electron densities calculated according to the LMTO-ASA (linearized muffin-tin orbital - atomic sphere approximation) approach. Sormann and Šob[34] remarked already that different ways of computing band structure lead to predicting different positron annihilation characteristics.

IV. CONCLUSIONS

In this work we tried on the simple example of lithium to find in a consequent many-body way (by solving in a non spherically symmetrical surrounding the appropriate nonlinear integro-differential equation derived on ground of the theory of liquids) deviations of local positron annihilation rates in a metal lattice from the local density approximation. We came to the conclusion that in lithium no drastic deviation from LDA occurs as concerns the annihilation rate. However, as concerns valence electrons, we observe a displacement of the node from 0.9 a.u. to 0.76 a.u., similar to that detected by Chiba in MgO[28]. We found also a deviation of the energy of electron-positron correlation from the local density approximation usually assumed in calculations. We found instead a term in the energy which we interpret as attraction of chemical character between the nucleus and the positron due to collectivization of core electrons.

So we computed the total positron annihilation rate in lithium using the local density approximation for the local annihilation rates. We used the numerical ATSUP code of Puska[33] for calculating positron wave functions, however, unlike Puska, we performed band structure calculations using the FLAPW code labelled WIEN95[30]. Moreover we added to the positron potential the term describing the positron-nucleus attraction as obtained in our calculations. As concerns jellium annihilation rates, we used the formula of Boroński and Nieminen[31]. In this way we obtained perfect agreement with experimental values and with the conclusions of Mijnarends *et al.*[14] concerning the LDA' model.

We confess that we are not very happy about this result. The formula of Boroński and Nieminen is the most frequently used in calculations trying to reproduce experimental data. Obviously it was found to give the best agreement. However, it is based on the calculations of Lantto which assume a Jastrow type trial function. This function neglects the momentum dependence of electron-positron scattering and the influence of the positron on electron-electron correlations. So we would have more confidence in calculations which take these effects, so well established in physics, into account. However, the annihilation rates obtained from them are obviously too high

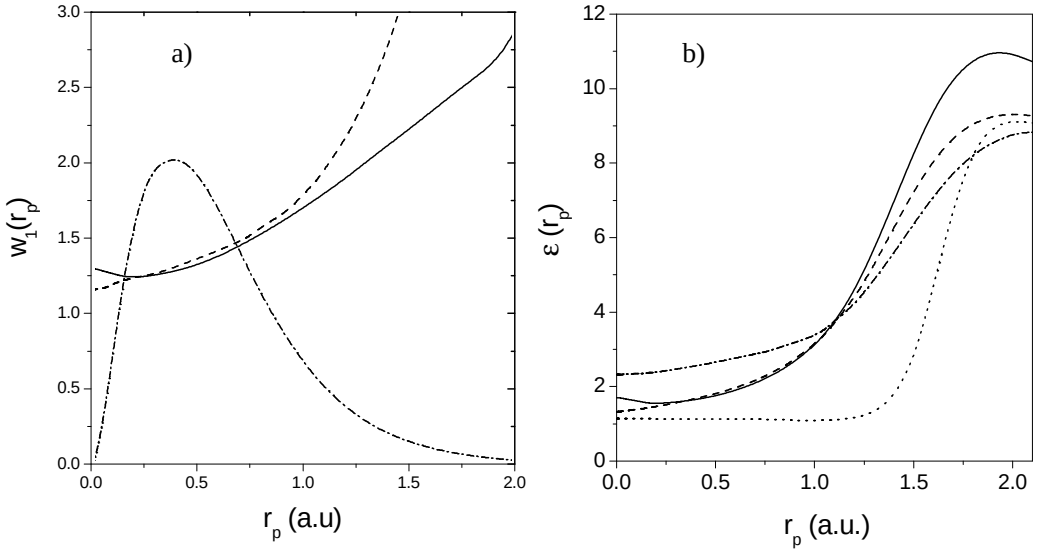

FIG. 3: a) The enhancement amplitude of core electrons in Li according to this work (full curve). The dashed curve shows the LPDA prediction. Additionally, the core electron distribution $4\pi r^2\psi_1^2(r)$ is plotted in arbitrary units (dashed-dotted curve). b) Effective enhancement $\varepsilon(r_p)$ inside an atom of lithium embedded in an electron gas calculated in this work (solid curve) and according to LDA (dashed curve), GGA (dotted curve) and WDA (dashed-dotted curve).

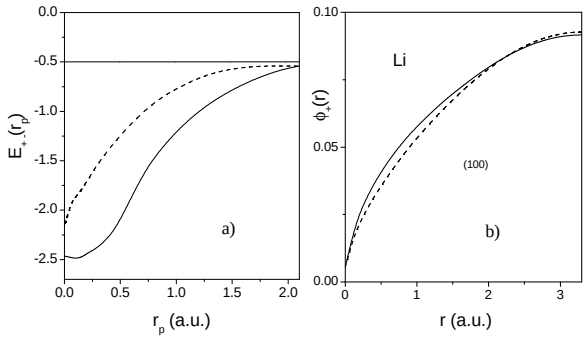

FIG. 4: a) Comparison of $E_{+-}(r_p) = 2E_1(r_p) + E_v$ in Li (full curve) and the energy of electron-positron correlation according to LDA (dashed curve). The energies have been normalized in such a way as to coincide at $r_p = 2.1$ a.u.
b) The positron density in Li along the (100) direction. The dashed curve was obtained while using the $e^+ - e^-$ correlation energy in LDA approximation. The full curve follows from including the effect of nucleus-positron attraction due to collectivization of core electrons.

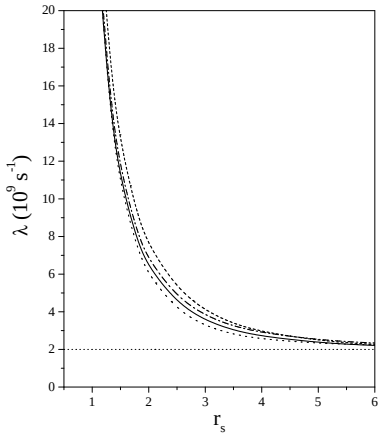

FIG. 5: Comparison of different formulas for the positron annihilation rate $\lambda(r_s)$ in an electron gas (dashed curve – Gondzik-Stachowiak[2], dashed-dotted curve – Barbiellini *et al*[1], solid curve – PHNC[25], dotted curve – Boroński-Nieminen[31]).

(Fig. 5). So we have to accept the Boroński-Nieminen formula as an expression poorly explained theoretically, but describing pretty well experimental data.

Among other results contained in the paper let us mention calculations of positron-nucleus attraction for Be, B, C, O and N due to collectivization of core electrons, of core enhancement for these elements (Appendix A) and description of the distribution of the electronic cloud screening the positron in different positions (Appendix B).

Acknowledgments

We are greatly indebted to Dr. M.J. Puska for making accessible to us his numerical code ATSUP for calculating positron wave functions.

APPENDIX A: POSITRON-CORE INTERACTION IN LIGHT ELEMENTS

For light elements heavier than beryllium the approach described by Eqs. (4) and (5) failed. Indeed, in boron it yielded $D = 0.59$ and collapsed in carbon where the condition (5) needed a value of D equal $2.5 \cdot 10^{-3}$. This, of course, is connected with the properties of valence electrons which are no longer itinerant. For this reason the condition (5) was replaced for boron, carbon, nitrogen and oxygen by the condition

$$4\pi \int_0^{cR_{WS}} r^2 dr \psi_2^2(r) + \frac{4}{3}\pi\rho_0(1-c^3)(R_{WS})^3 = Z - 2 \tag{A1}$$

while in Eq. (A1) the role of R_{WS} is played now by cR_{WS}. The normalization condition for ψ_1 is the usual one. Note that the dependence of IPC characteristics on the values of D and c in Eqs. 4 and (A1) is negligible. Our calculations show that the enhancement amplitude for core electrons in Be, B, C, O and N is even lower from the LDA curve than the corresponding figure for Li. In general, however, its behavior is quite similar to that shown in Fig. 3a. Unfortunately, the effective enhancement for those elements could not be computed for reasons explained in Section II.

As concerns the energies of positron-electron correlation for Be, B, C, O and N the effect of core electron collectivization leads to an attraction between the positron and the nucleus. The effect is bigger for increasing atomic mass of the element.

APPENDIX B: THE DENSITY AMPLITUDE $\chi_2(\mathbf{r}_p, \mathbf{r})$

Fig. 6 shows the change of the density amplitude $\chi_2(\mathbf{r}_p, \mathbf{r}) - \psi_2(\mathbf{r})$ for $\mathbf{r}$ along the line connecting the nucleus and the positron and r_p equal a) 0.3 and b) 1.8 . Fig. 7 shows the behavior of the screening cloud $\chi_2^2(\mathbf{r}_p, \mathbf{r}) - \psi_2^2(\mathbf{r})$ for the same values of $\mathbf{r}$ and $\mathbf{r}_p$. One should remember that the corresponding density amplitude changes sign when crossing the node, and this feature persists in the presence of the positron. Moreover, the node is shifted by the positron. It is striking that the highest density of the screening cloud occurs close to the nucleus even for the positron well beyond the node region of the density amplitude. This suggests that our figures are less reliable for the positron in the interstitial region, since the screening cloud extends over several atomic cores and these facts are not included in our model.

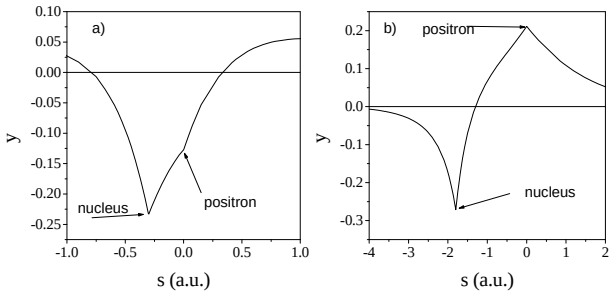

FIG. 6: $\chi_2(\mathbf{r}_p, \mathbf{s} + \mathbf{r}_p) - \psi_2(\mathbf{s} + \mathbf{r}_p)$ in Li for r_p equal a) 0.3 b) 1.8 . $\mathbf{s}$ is taken along the line connecting the nucleus and the positron.

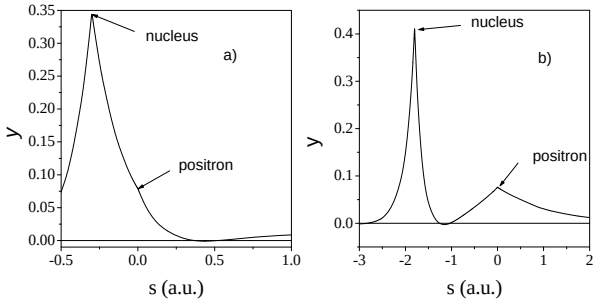

FIG. 7: The screening cloud distribution in Li around a positron at r_p equal a) 0.3, b) 1.8 . $\mathbf{s} = \mathbf{r} - \mathbf{r}_p$ is taken along the line connecting the nucleus and the positron.

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